

2-Methylhexane  
591-76-4 | DTXSID5052256

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** -114 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 1.00

**Confidence level:** 9.12e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

3-Methylhexane

**Measured:** -119

**Predicted:** -114

[Image not found](#)

2-Methylhexane

**Measured:** -118

**Predicted:** -114

[Image not found](#)

Pentane, 3-ethyl-

**Measured:** -119

**Predicted:** -116

[Image not found](#)

2-Methylheptane

**Measured:** -109

**Predicted:** -110